Three-Dimensional Spin Rotations at the Fermi Surface of a Strongly Spin-Orbit Coupled Surface System

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Abstract: The spin texture of the metallic two-dimensional electron system ($\sqrt{3}\times\sqrt{3}$)-Au/Ge(111) is revealed by fully three-dimensional spin-resolved photoemission, as well as by density functional calculations. The large hexagonal Fermi surface, generated by the Au atoms, shows a significant splitting due to spin-orbit interactions. The planar components of the spin exhibit a helical character, accompanied by a strong out-of-plane spin component with alternating signs along the six Fermi surface sections. Moreover, in-plane spin rotations toward a radial direction are observed close to the hexagon corners. Such a threefold-symmetric spin pattern is not described by the conventional Rashba model. Instead, it reveals an interplay with Dresselhaus-like spin-orbit effects as a result of the crystalline anisotropies.

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Supplemental Material

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This supplemental material provides details of the band-structure modeling according to Eq. (3):

$$H(k) = \left(\frac{\hbar^2 k^2}{2m^*} - C + c_h(k_+^6 + k_-^6)\right)\sigma_0 + v(k_x\sigma_y - k_y\sigma_x) + \lambda(k_+^3 + k_-^3)\sigma_z + i\zeta(k_+^5\sigma_+ - k_-^5\sigma_-),$$

where σ_0 is the 2×2 identity matrix, σ_x, σ_y and σ_z are Pauli matrices, $\sigma_\pm = \sigma_x \pm i\sigma_y$, and $k_\pm = k_x \pm ik_y$. This Hamiltonian is invariant with respect to symmetry operations of the C_{3v} group and time-reversal symmetry. For the following choice of parameters, the $E = 0$ energy surface of this model Hamiltonian reproduces well both, the Fermi contour and the spin structure of the metallic surface band in $(\sqrt{3}\times\sqrt{3})$-Au/Ge(111): $m^* = 0.4\,m_e$, $C = 0.77\,\mathrm{eV}$, $c_h = 70\,eV\mathring{A}^{-6}$, $v = -0.1\,eV\mathring{A}^{-1}$, $\lambda = -7\,eV\mathring{A}^{-3}$, $\zeta = 5.5\,eV\mathring{A}^{-5}$.

The first part of the Hamiltonian, proportional to σ_0, is the spinless part, giving rise to spin doubly degenerate states. The sixth-order in k term in the parentheses is responsible for the hexagonal warping of the constant energy contours. This term reproduces well the Fermi contour of our *ab-initio* calculations, before including the spin-orbit interaction.

The second part of the Hamiltonian, $v(k_x\sigma_y - k_y\sigma_x)$, is the well-known Rashba term. It has full $O(2)$ symmetry and produces an isotropic spin splitting. The two resulting constant-energy contours (corresponding to $\mathrm{S1_A}$ and $\mathrm{S1_B}$) have a spin texture being fully planar, vortical (clockwise for $\mathrm{S1_B}$ and counter-clockwise for $\mathrm{S1_A}$) and perpendicular to the surface momentum vector (k_x, k_y).

The third part of the Hamiltonian, of third-order in k, was proposed by L. Fu in Ref. 24 in order to explain the hexagonal warping of the Dirac-fermion band at the surface of the topological insulator $\mathrm{Bi_2Te_3}$. Apart from affecting the shape of energy contours, it generates a z-component in the spin vector. This vertical part of the spin exhibits an alternating sign (*up* or *down*) between neighboring hexagonal sheets of the energy contours. The in-plane part of the spin vector remains, however, perpendicular to the momentum vector (k_x, k_y). Along the $\overline{\Gamma}-\overline{\mathrm{K}}$ azimuth, there is no z-component of spin due to symmetry reasons.

The last term, of fifth-order in k, $i\zeta(k_+^5\sigma_+ - k_-^5\sigma_-)$, was recently proposed by S. Basak *et al.* [25]. This term is needed to explain the *ab-initio* results showing radial rotations of the in-plane spin components for the Dirac-fermion bands at the surface of the topological insulator $\mathrm{Bi_2Te_3}$. Similarly as the third-order term, it contributes to the hexagonal warping of the energy contours, but its main function is the rotation of in-plane spin components towards a radial direction. This happens in close vicinity to the $\overline{\Gamma}-\overline{\mathrm{K}}$ azimuth.

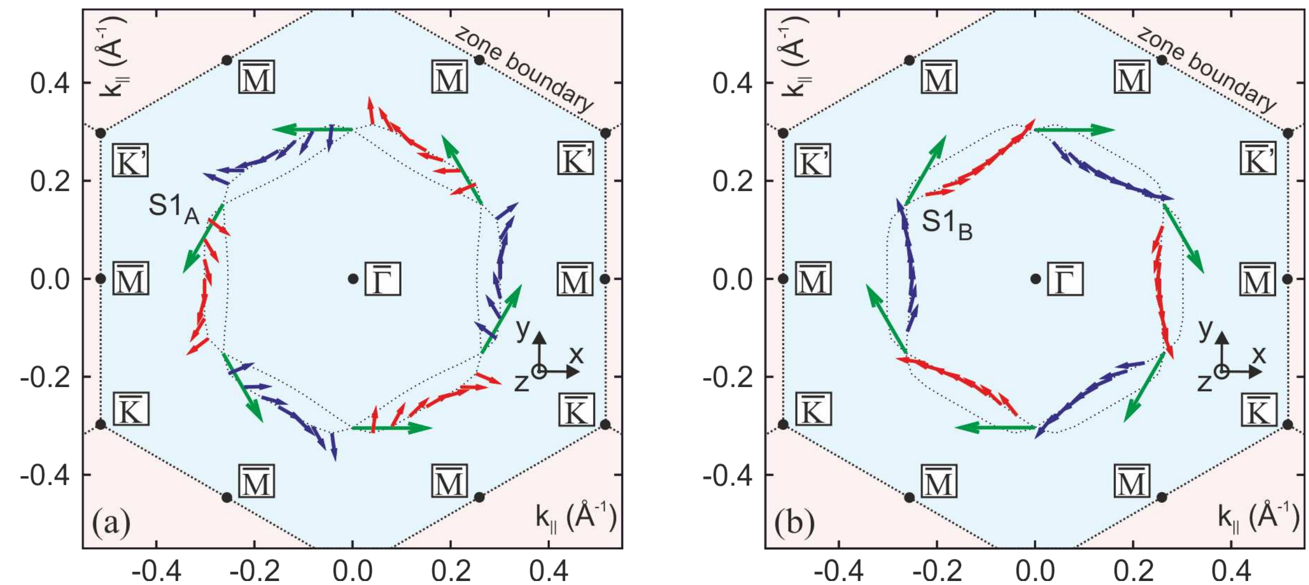

Figure S1: $E = 0$ energy contours derived from the model Hamiltonian with the in-plane spin texture of the spin-split states (a) $S1_A$ and (b) $S1_B$. The spin arrows are red for spins directed out-of-plane and blue for an orientation into the plane. Green color signifies fully in-plane spin alignment.

Figure S1 displays the energy contours and spin texture of the model Hamiltonian (Eq. (3)) for the choice of parameters listed above. For better clarity each spin-split state ($S1_A$ and $S1_B$) is shown in a separate plot.